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Modeling of the wrinkling of premixed turbulent flames in the thin reaction zones regime for large eddy simulation

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Large eddy simulations (LES) have been successfully applied to premixed turbulent flames in the flamelet regime. However, comparatively little effort to date has focussed on modelling of premixed flames for LES in regimes of combustion in which the small turbulence scales can penetrate the flame, the most important of which is the so-called thin-reaction zones regime. Utilizing concepts of fractal geometry and Damköhler's limiting flame-speed scalings, this paper proposes a new flame wrinkling model which is intended to be applicable in such regimes. *A priori* analysis of direct numerical simulations of turbulent, premixed, methane-air slot-jet flames are used to assess the model as well as three literature models of the flame wrinkling. The models are all implemented in a constant coefficient version and in a dynamic version using an approximate Germano identity. We investigated the performance of the models as filter size and downstream distance are varied, and good results are obtained for a range of filter sizes.

1. Introduction

Premixed turbulent combustion is a problem of considerable practical significance, for example in stationary power gas turbines, spark-ignition engines, and explosions. Much effort has therefore been devoted to its modelling (Peters 2000; Veynante & Vervisch 2002). Recently, LES have emerged as the next-generation approach to improve this modelling via direct resolution of the large, energy-containing scales of fluid motion (Pitsch 2006).

The closure of the nonlinear chemical source term then appears as the central modelling challenge. This closure has been dealt with in several different ways, for example, using a level-set equation (Pitsch 2005; Knudsen & Pitsch 2008), a flame surface density concept (Hawkes 2000; Hawkes & Cant 2001; Knikker *et al.* 2002) or an artificially thickened flame approach (Colin *et al.* 2000; Charlette *et al.* 2002*a*,*b*). Although the implementation details of these approaches are different, they all revolve around a central concept that the chemical length-scales are thin relative to turbulence length-scales. With this assumption, the modelling challenge may be decomposed into the problem of determining the unresolved surface area of the thin flame front, and the burning rate per unit area of that surface. This paper focusses on the former issue whereas the latter is outside the scope.

The above-mentioned models, with the exception of those due to Pitsch, are principally intended for, and have been principally assessed within, the flamelet regime of premixed

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combustion. In this regime, all length-scales of turbulence are larger than the thermal flame thickness and the Karlovitz number, Ka, is less than unity. However, as pointed out by Peters (2000), in many practical devices a situation exists where Ka $>$ 1 and turbulence can penetrate and disrupt the preheat zone of the flame, but not the thinner reaction zone: the "thin reaction-zones" regime. There have been comparatively fewer assessments of the models for Ka $>$ 1, and also very few direct comparisons between different models against the same data set. This work is intended to help address these gaps.

This article proposes a new flame wrinkling model based on a fractal concept. There exists a wealth of experimental data that show a power-law dependence of the measured flame area with the measurement resolution over a range of measurement resolutions (Gouldin *et al.* 1988; Mantzaras *et al.* 1989; Gülder 1991; Knikker *et al.* 2002). Adopting the terminology of fractal geometry, this range of measurement resolutions is bounded by the inner cut-off η_i, which is physically interpreted as the smallest scale of flame wrinkling, and the outer cut-off η_o, which is physically interpreted as the largest scale of flame wrinkling. For LES, the power-law dependence provides an elegant way of incorporating the filter-size dependence of the flame wrinkling into a model. This approach appears to have been first suggested by Lipatnikov & Chomiak (1999), who argued for the Gibson scale as an inner cut-off (Peters 2000) and employed an empirical correlation for the fractal dimension, D_f. Knikker *et al.* (2002) used experimental measurements of η_i and β to provide *a priori* assessments of a scale-similarity model for the flame surface density. Charlette *et al.* (2002*a*,*b*) provided an analysis leading to a model for flame wrinkling that is implemented using a dynamic approach in the context of the thickened flame model. Fureby (2005) used a very similar model to that of Charlette *et al.* (2002*a*) for the inner cut-off, but applied the model using a flame-wrinkling formulation.

All the above works focussed only on the flamelet regime. Here, an attempt is made to provide an unified model for flame wrinkling for the corrugated flamelets regime and the thin reaction zones regime from a power-law perspective. The new approach is motivated by the fact that if a power law practically exists, the invariance of the Karlovitz number in the inertial range together with Damköhler's limits (Damköhler 1940) can be used to derive the fractal dimension and inner cut-off. It is hoped that this approach could lead to a reduction of undesirable filter-size dependencies of the modelling outcomes.

A direct numerical simulation (DNS) data set has been used to assess the new model and three other models from the literature (Pitsch 2005; Charlette *et al.* 2002*b*; Colin *et al.* 2000) in *a priori* tests. The DNS data from (Sankaran *et al.* 2007; Chen *et al.* 2009) model a set of three-dimensional spatially evolving turbulent premixed Bunsen flames. The Bunsen flame offers two important advantages for model validation over the freely propagating flames that have been typically studied. First, the flame is statistically stationary whereas freely propagating flames are frequently not. Second, the presence of mean shear supports turbulence such that higher levels are obtainable.

The paper is organized as follows. Section 2 presents the proposed flame wrinkling model. Section 3 presents the approaches from the literature with which the model will be compared. Section 4 presents a dynamic implementation of the models. Section 5 briefly outlines the DNS. Results are presented in section 6 and conclusions in section 7.

2. Fractal model development

The flame wrinkling factor Ξ for LES represents the ratio of the total flame area to the resolved flame area. Starting from a progress variable c having the value zero in reactants and unity in products, one definition that has been employed by several groups is in terms of a generalized flame surface density:

$$\Sigma = \overline{|\nabla c|}, \tag{2.1}$$

where $\overline{(\ldots)}$ represents the LES filtering operation. Then,

$$\Xi = \frac{\overline{|\nabla c|}}{|\nabla \overline{c}|} = \frac{\Sigma}{|\nabla \overline{c}|}. \tag{2.2}$$

The basic form of a fractal model for LES was given by Charlette *et al.* (2002*a*):

$$\Xi = \left(1 + \frac{\Delta}{\eta_i}\right)^{\beta}, \tag{2.3}$$

where η_i is the inner cut-off scale representing the smallest scale of flame wrinkling, Δ is the LES filter size (which is presumed to be the outer cut-off scale), and β is the scaling exponent which is related to the fractal dimension by $D_f = 2 + \beta$.

It is noted that η_i and β are supposed to be physical rather than numerical quantities and should therefore be modelled as invariant with respect to the filter size, if possible. Both Charlette *et al.* (2002*a*) and Fureby (2005) determined the inner cut-off scale from a balance of total sub-grid area production and destruction. If an inertial range scaling of the turbulence intensity is assumed, this choice leads to an estimate of the inner cut-off that is filter size-dependent. Fureby's fractal dimension is also filter size-dependent. Changes of these parameters with filter size are possible if the flame has a multi-fractal-type behavior but should only occur if there is a "regime change" of the unresolved versus resolved physics (Pitsch 2005). However, these models will lead to a filter size-dependence without any regime change. This motivates the development of a model that is theoretically filter size-independent within an inertial range.

Damköhler (1940) used basic physical reasoning to show that in the flamelet regime, the turbulent burning speed, s_T, scales with the turbulence intensity u' (Damköhler's large-scale limit), whereas in the distributed reaction regime it scales with the square root of the turbulent diffusivity divided by the chemical time-scale (Damköhler's small-scale limit). Pitsch (2005) extended this concept to LES, drawing on prior work in the context of Reynolds-averaging by Peters (2000). For this short article, we simply assume these limits apply. We have developed additional physical arguments to support this limit but these must be relegated to future work. We also assume there is no regime change in terms of the nature of the represented resolved versus unresolved physics.

If the inner cut-off is filter size-invariant within the inertial range, it can only be a function of flame parameters and the turbulent kinetic energy dissipation rate. Therefore Karlovitz number is the relevant dimensionless parameter, and we model

$$\eta_i/\delta_L \sim \mathrm{Ka}^a, \tag{2.4}$$

where a is to be determined. Following Peters (2000), Ka can be expanded in terms of the sub-grid turbulence intensity u'_Δ, laminar flame speed s_L and thickness δ_L defined as D/s_L. For Damköhler's large-scale limit it may be shown that for high wrinkling

$$\Xi \sim \left(\frac{u'_\Delta}{s_L}\right) \sim \left(\frac{u'_\Delta}{s_L}\right)^{\frac{-3a}{2}\beta} \left(\frac{\Delta}{\delta_L}\right)^{(1+\frac{a}{2})\beta}. \tag{2.5}$$

The scaling shows that $a = -2$ and $\beta = 1/3$. This leads to $D_f = 7/3$ for the fractal dimension, and the Gibson scale as the inner cut-off $\sim L_G = (s_L/u'_\Delta)^3 \Delta$. Although this derivation is different, L_G has been previously proposed for the inner cut-off in the flamelet regime (Peters 2000; Kerstein 1988). The choice $D_f = 7/3$ has also been advocated by others (Kerstein 1988; Sreenivasan 1991; Gouldin 1988).

Using a similar procedure for Damköhler's small-scale limit leads to $a = -1/2$ and $\beta = 2/3$, and hence $\eta_i \sim \eta_{\mathrm{OC}} = (D^3/\epsilon)^{1/4}$ (the Obukov-Corrsin scale). The fractal dimension is found to be $D_f = 8/3$. This limit corresponds to high Karlovitz number and thus, ignoring significant heat release effects, a flame behaves like a passive scalar (Peters 2000). Therefore it is physically clear that a scale of the order of the Obukov-Corrsin scale, *i. e.* , order of the Kolmogorov scale (η), is the appropriate length scale of flame wrinkling. Some experiments have provided support for this finding (Gülder 1991; Gülder & Smallwood 1995). Also, other researchers have proposed the Kolmogorov scale as an inner cut-off (Gouldin 1987; Gülder 1991) (but have used different fractal dimensions). The value $D_f = 8/3$ has not previously been proposed to our knowledge in the context of premixed flames; however, it was proposed by Mandelbrot (1975) for nonreacting flows assuming Gauss-Kolmorogov turbulence.

The transition of the fractal dimension between regimes is not immediately obvious, since arguably the large scales (at which the fractal dimension is apparent) should be independent of the mechanism of dissipation of the small scales. However, this paradox has been resolved by Constantin *et al.* (1991), who studied variations of the fractal dimension of scalar concentration iso-surfaces in non-reacting jets. Their experiments showed that for low values of the concentration, which correspond to the outer jet region where external intermittency dominates, that the fractal dimension was $\sim 7/3$, while for higher values inside the fully turbulent region of the jet, the fractal dimension was $\sim 8/3$. This was explained by the fact that in the well-mixed region, the probability of observing a given iso-surface crossing diminishes with decreasing scale at a faster rate since the fluctuations associated with that length scale are also diminishing.† Here we identify the regime which has a behavior akin to outer-scale intermittency as the flamelet regime (and Damköhler's large-scale limit), while the inner well-mixed region is identified with Damköhler's small-scale limit. This identification may go some way to explain why fractal dimension is observed experimentally to increase with increasing turbulence intensity in premixed flames.

To obtain a practically usable model between these limits, we simply chose functions that transition smoothly between the identified high and low Karlovitz number limits. The exponent β is expressed as

$$\beta = D - 2 = \frac{1}{3} + \frac{1}{3}\frac{(\eta_{oc}/b)^x}{(L_G/a)^x + (\eta_{oc}/b)^x}, \tag{2.6}$$

while the inner cut-off scale η_i is fitted as

$$\eta_i = ((L_G/a)^x + (\eta_{oc}/b)^x)^{1/x}. \tag{2.7}$$

The constants a, b and x are model parameters. The values were chosen to provide a

† We are grateful to Alan Kerstein for a very helpful discussion that clarified these points.

good match to one of the DNS cases, with a filter size of $11dx$ (where dx is DNS grid spacing), resulting in $a = 2.0$, $b = 0.145$, and $x = 4$. The parameters were kept fixed for the other cases and filter sizes. A dynamic approach to obtain the value of β was also developed, as discussed in section 4.

3. Literature models

The proposed model is compared with the models of Colin *et al.* (2000), Charlette *et al.* (2002*b*) and Pitsch (2005).

Colin *et al.* (2000) modelled the flame wrinkling as

$$\Xi = 1 + \beta \frac{2\ln 2}{2C_{\mathrm{ms}}(\mathrm{Re}_t^{1/2} - 1)} \Gamma_k \left(\frac{\Delta}{\delta_L}, \frac{u'_\Delta}{s_L} \right) \frac{u'_\Delta}{s_L}, \tag{3.1}$$

where Re_t is global Reynolds number, the function Γ_k is an efficiency function obtained from DNS of two-dimensional flame-vortex interactions and is given in Colin *et al.* (2000), and C_{ms} is a constant.

Charlette *et al.* (2002*a*,*b*) modelled flame wrinkling based on a fractal concept as

$$\Xi = \left(1 + \min \left(\frac{\Delta}{\delta_L^0}, \Gamma_k \left(\frac{\Delta}{\delta_L^0}, \frac{u'_\Delta}{s_L} \right) \frac{u'_\Delta}{s_L} \right) \right)^{\beta}, \tag{3.2}$$

where δ_L^0 is computed from $\delta_L^0 s_L / \nu = 4$.

Pitsch (2005) has modelled the flame speed as

$$\Xi = 1 - \frac{b_3^2 c_\nu c_s \Delta s_L}{2 b_1 Sc_t D} + \sqrt{\left(\frac{b_3^2 c_\nu c_s \Delta s_L}{2 b_1 Sc_t D} \right)^2 + \frac{b_3^2 \nu_t}{Sc_t D}}, \tag{3.3}$$

where ν_t is the sub-grid turbulent viscosity, Sc_t is the turbulent Schmidt number, D is the molecular diffusivity, and $c_\nu c_s$ is a Smagorinsky-type constant. The constants b_1 and b_3 were originally estimated based on total turbulent flame speed measurements (*i. e.* , for Reynolds-averaging). We found that these values over predicted the flame wrinkling when compared with this data set, and there is no reason to suppose the constants should be the same for LES and Reynolds-averaging, so the parameters were adjusted to have values 1.0 and 0.15, respectively, to provide a good fit for case C with a filter size of 11 DNS grid points, but kept the same for the other filter sizes. The value for b_1 that we used is consistent with the range 0.5 to 1.5 which was found using a dynamic implementation of this model due to Knudsen & Pitsch (2008).

4. Approximate Germano identity

A dynamic Germano-type method Germano *et al.* (1991) has been employed to calculate model coefficients locally. Let $\Xi_m(u'_\Delta, \Delta)$ be the model for flame wrinkling. Now, the classic Germano equation for the flame surface density may be stated as Hawkes (2000)

$$\widehat{\overline{|\nabla c|}} = \Xi_m(u'_{\hat{\bar{\Delta}}}, \hat{\bar{\Delta}}) \left| \nabla \hat{\bar{c}} \right| = \widehat{\Xi_m(u'_{\bar{\Delta}}, \bar{\Delta}) \left| \nabla \bar{c} \right|}, \tag{4.1}$$

where $\widehat{(\ldots)}$ represents the test-filtering operation.

When estimating the flame surface density using the standard Germano approach above there are three difficulties. The first is that if the test filter does not include the resolved flame surface, the Germano equation cannot provide the constant. The second is that some of the model equations are nonlinear in the parameter, which in principle would involve a nonlinear solution strategy over the test filter. The final difficulty is that it is likely that some form of averaging of the obtained parameters is necessary. To circumvent these difficulties, we propose an approximate Germano equation using a resolved surface-weighted averaging procedure as follows. We define surface averages, weighted by the resolved flame surface area at the different levels for a quantity q, as

$$\langle q\rangle_{\hat{\hat{s}}} = \frac{\langle q\,|\nabla\hat{\bar{c}}|\rangle}{\langle|\nabla\hat{\bar{c}}|\rangle}, \quad \text{and } \langle q\rangle_{\hat{s}} = \frac{\widehat{\langle q\,|\nabla\bar{c}|\rangle}}{\widehat{\langle|\nabla\bar{c}|\rangle}}. \tag{4.2}$$

With these definitions, the simplified Germano equation is

$$\widehat{\langle\overline{|\nabla c|}\rangle} = \Xi_m(\langle u'_{\hat{\bar{\Delta}}}\rangle_{\hat{\hat{s}}}, \hat{\bar{\Delta}})\langle|\nabla\hat{\bar{c}}|\rangle = \Xi_m(\langle u'_{\bar{\Delta}}\rangle_{\hat{s}}, \bar{\Delta})\widehat{\langle|\nabla\bar{c}|\rangle}. \tag{4.3}$$

In the present article we take the operator $\langle\ldots\rangle$ to be a spatial average in the homogeneous direction, followed by a spatial integration across the jet. Therefore the coefficients vary only in the streamwise direction and in time. The parameter β in Equations 2.3, 3.1, and 3.2 was taken as the free parameter to be determined dynamically. For Pitsch's model, we took the parameter b_3 as the free parameter to be determined dynamically. The reason for the difference from Knudsen & Pitsch (2008), who took the free parameter as b_1, is that the DNS lie on the upper boundary of the thin reaction zones regime and it is expected that Damköhler's small-scale limit applies rather than the large-scale limit. All the models except that of Pitsch (2005) had a closed-form solution for the free parameter. For this model we used a Newton iteration to determine the parameter.

5. DNS Data

The DNS corresponds to a spatially developing turbulent Bunsen flame configuration. Full details are given elsewhere (case C in Chen *et al.* (2009)). There is a central planar jet of premixed fuel and air at 100 m/s which is surrounded on either side by a co-flow at 25 m/s having temperature and composition of the adiabatic burned products of the reactant jet. Figure 1 shows an instantaneous iso-surface of reaction progress variable defined based on normalized oxygen mass fraction and demonstrates the configuration. Referring to this figure, periodic boundary conditions were specified on the $x-y$ boundary planes while non-reflecting outflow boundary conditions were specified on the $y-z$ and $x-z$ boundaries. The flame was anchored at the inflow boundary by specifying the temperature and species profiles from an unstrained laminar flame solution, and a random velocity field was imposed that satisfies continuity and has prescribed length scales.

The chemistry was treated using a reduced methane-air kinetic mechanism (Sankaran *et al.* 2007). The unstrained laminar flame properties at these conditions are s_L=1.8 m/s and the laminar flame thickness based on maximum temperature gradient is $\delta_T = 0.3$ mm. The central reactant jet of premixed methane and air has an equivalence ratio of 0.7 and a temperature of 800 K. The jet Reynolds number based on the inlet center-line velocity and the slot-width is $\mathrm{Re}_{\mathrm{jet}} = 2100$ and the inlet turbulence intensity is u'=33m/s.

The simulation was performed using Sandia DNS code, S3D, which solves the fully compressible Navier-Stokes, species and energy equations with high-order methods (Chen *et al.* 2009). A uniform grid spacing (dx) of 20 μm is used in the streamwise and spanwise

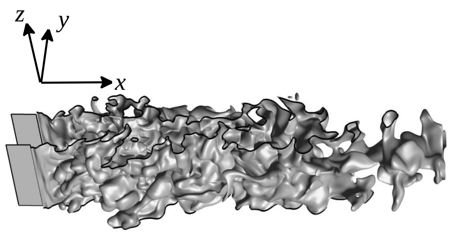

FIGURE 1. The isosurface of progress-variable 0.65, in case C.

directions, while an algebraically stretched mesh is used in the transverse direction, with a uniform mesh in the core region of interest. There are ~ 15 grid points across δ_T.

To assess the performance of the models, an *a priori* test was conducted. The DNS data were filtered with a top-hat filter, and the model predictions of the flame surface area based on the sub-grid turbulence intensity from the DNS were compared with the actual flame surface area.

6. Results

The models are now compared on a statistical basis. The LES-filtered results for flame surface density were Reynolds averaged, which involves averaging over the homogeneous spanwise direction and in time and exploiting symmetry in the transverse direction. These results were then integrated over the transverse direction (y), which corresponds to an average "flame surface area ratio" (Peters 2000), and plotted as a function of the streamwise coordinate (x).

Figure 2 a-c (the left column) shows the predictions of the models and the DNS result against the streamwise distance x normalized by the jet half-height, H. Figure 2 a-c shows results with a filter size of 5, 11, and 21 dx, which corresponds to $\Delta/\delta_T = 0.33$, 0.73 and 1.4, $\Delta/\eta = 6.35$, 13.97 and 26.67 and $\ell_T/\Delta = 36$, 16.36 and 8.57, respectively, where ℓ_T is integral length scale and all parameters are computed from inflow values. The filter size of $11dx$ is probably most representative of LES in the sense that it resolves approximately 80% of the turbulent kinetic energy in the inflow region.

The models all offer a good qualitative match to the DNS, and the trends with downstream distance are well captured. As a consequence of increasing resolution of the flame wrinkling, the performance improves with both decreasing filter size and increasing downstream distance. The proposed model and that of Pitsch (2005) slightly overpredict the flame surface area ratio for small filter sizes, and slightly underpredict it for large filter sizes. Considering the present model has been developed with intent to be filter size-invariant, we are encouraged by the good performance with respect to filter size variation. The model of Colin *et al.* (2000) consistently overpredicts the DNS, whereas the Charlette *et al.* (2002*a*) model underpredicts . However, note that both the Pitsch and proposed models had the constants adjusted to match the $11dx$ case. The other two models were developed with the aid of other DNS databases, which may explain their good performance without adjustment.

The arbitrary adjustment of model constants is of course undesirable, therefore we investigated a dynamic procedure, which was explained in section 4. For each model, except that of Pitsch for the reasons described in section 4, one model parameter coefficient was

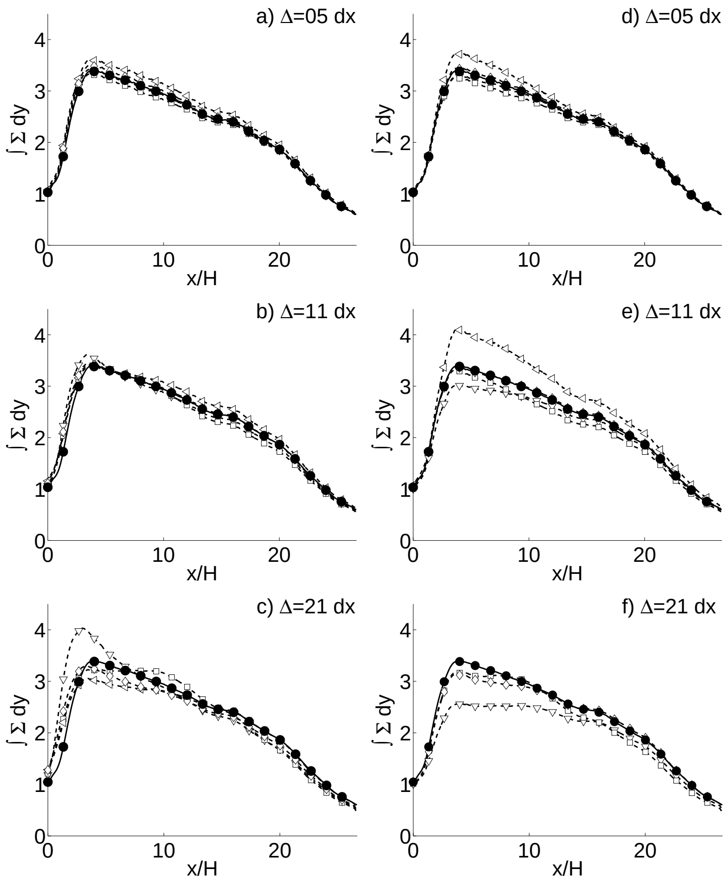

FIGURE 2. $\int \Sigma dy$, for DNS and models. Left : Constant coefficients; Right : Dynamic coefficients. Legend: (●) DNS; (◇) Proposed model; (▷) Pitsch; (▽) Colin (□) Charlette

computed dynamically and the results are compared in Figure 2 d-f. The results were variable. Performance deteriorated for the Pitsch model, and in fact no root of the Germano equation existed for the 21 dx case. The dynamic approach marginally improved the results from Colin *et al.* (2000). Significantly improved results were obtained for both power law-based models, the one due to Charlette *et al.* (2002*b*) and the proposed fractal model, which is nearly indistinguishable from the DNS result for the filter size $11dx$. The performance of all the models begins to break down at 21 dx but this filter size is larger than is typical of LES in terms of kinetic energy resolution.

7. Conclusions

Damköhler's scaling arguments for the turbulent flame speed were used with a fractal concept to develop a model for flame wrinkling. In order to design a model that is filter size-invariant in the inertial range, it was argued that the inner cut-off and fractal dimension can only be functions of Karlovitz number and flame parameters. Dimensional reasoning and Damköhler's limiting scalings were then used to infer these values in the limiting regimes. The model was further elaborated by development of an approximate

Germano-type equation based on resolved-scale surface-weighted averaging, which enables the dynamic determination of one model parameter.

Data from DNS of a turbulent premixed Bunsen flame has been analyzed to assess the performance of the new model and compare it to three models from the literature. All of the models are found to be able to quantitatively predict the DNS-observed trends with filter size and downstream distance, and the quantitative agreement is good except at very large filter sizes. The results for the dynamic versions of the models were mixed with deteriorated performance for the Pitsch model, and improved for the other three models, and notably the two models based on power-law approaches, *i. e.* , Charlette *et al.* (2002*b*) and the present model. The performance of the proposed model is noted to be particularly promising with respect to changes in filter size.

Ongoing work is examining the other cases available in Chen *et al.* (2009), and aims to conduct *a posteriori* tests using the level-set approach (Knudsen & Pitsch 2008).

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